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2-Aminobenzoic acid–4,4′-bipyridine (2/1)

Hadi D. Arman[a] and Edward R. T. Tiekink[b]*

[a]Department of Chemistry, The University of Texas at San Antonio, One UTSA Circle, San Antonio, Texas 78249-0698, USA, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: edward.tiekink@gmail.com

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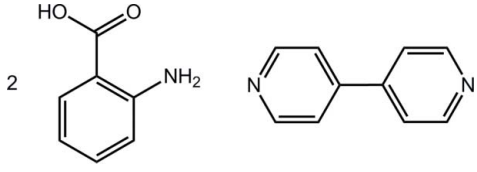
Key indicators: single-crystal X-ray study; T = 98 K; mean σ(C–C) = 0.003 Å; R factor = 0.061; wR factor = 0.159; data-to-parameter ratio = 15.1.

The asymmetric unit of title co-crystal, $C_{10}H_8N_2{\cdot}2C_7H_7NO_2$, comprises a centrosymmetric 4,4′-bipyridine molecule, and a 2-aminobenzoic acid molecule in a general position. The latter is effectively planar [C—C—C—O torsion angle = 5.0 (3)°] owing to an intramolecular N—H···O(carbonyl) hydrogen bond. Three-molecule aggregates are formed *via* O—H···N(pyridyl) hydrogen bonds and these are connected into supramolecular layers in the *bc* plane by N—H···O(carbonyl) hydrogen bonds and π–π interactions between pyridyl and benzene rings [inter-centroid distance = 3.634 (2) Å]. Layers are connected along the *a* axis by weak π–π interactions between benzene rings [3.964 (2) Å].

Related literature

For co-crystals of 2-aminobenzoic acid with pyridyl derivatives, see: Arman, Kaulgud *et al.* (2012); Arman, Miller & Tiekink (2012).



Experimental

Crystal data

$C_{10}H_8N_2{\cdot}2C_7H_7NO_2$
M_r = 430.46
Monoclinic, $P2_1/c$
a = 10.782 (5) Å
b = 10.998 (5) Å
c = 8.951 (4) Å
β = 107.215 (7)°
V = 1013.9 (8) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 98 K
0.46 × 0.11 × 0.09 mm

Data collection

Rigaku AFC12/SATURN724 diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.723, T_{max} = 1.000
7849 measured reflections
2320 independent reflections
1932 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
Standard reflections: 0

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.159
S = 1.11
2320 reflections
154 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1n···O2	0.88 (1)	2.02 (2)	2.697 (2)	132 (2)
O1—H1o···N2^{i}	0.85 (1)	1.81 (1)	2.655 (2)	174 (2)
N1—H2n···O2^{ii}	0.88 (2)	2.14 (2)	3.002 (3)	170 (2)

Symmetry codes: (i) $x, y, z+1$; (ii) $x, -y+\frac{3}{2}, z-\frac{1}{2}$.

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2276).

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supplementary materials

Acta Cryst. (2013). E**69**, o1447 [doi:10.1107/S160053681302271X]

2-Aminobenzoic acid–4,4′-bipyridine (2/1)

Hadi D. Arman and Edward R. T. Tiekink

1. Comment

The title co-crystal, (I), was formed in continuation of on-going structural studies of co-crystals involving 2-amino-benzoic acid with various pyridyl derivatives (Arman, Kaulgud *et al.*, 2012; Arman, Miller & Tiekink, 2012).

The asymmetric unit contains a molecule of 2-aminobenzoic acid in a general position, and half a molecule of 4,4′-bi-pyridine disposed about a centre of inversion, Fig. 1. The carboxylic acid is planar owing to the presence of an intramolecular N1—H···O2 hydrogen bond, Table 1, as seen in the C1—C2—C7—O2 torsion angle of 5.0 (3)°. The acid and base associate into a centrosymmetric three-molecule aggregate *via* O1—H···N2 hydrogen bonds, Fig. 2 and Table 1. These assemble into columns along the *c* axis *via* *π*—*π* interactions between the pyridyl and benzene rings [inter-centroid distance = 3.634 (2) Å], Fig. 2. Supramolecular layers in the *bc* plane are formed by N1—H···O2 hydrogen bonds, Table 1. Connections between layers along the *a* axis are weak *π*—*π* interactions between benzene rings [inter-centroid distance = 3.964 (2) Å for symmetry operation: -*x*, - *y* + 1, -*z* + 1] (Fig. 3.)

2. Experimental

Crystals of (I) were obtained by the co-crystallization of 2-aminobenzoic acid (Sigma-Aldrich, 0.18 mmol) and 4,4′-bi-pyridine (Sigma-Aldrich, 0.14 mmol) in chloroform solution. Crystals were obtained by slow evaporation.

3. Refinement

C-bound H-atoms were placed in calculated positions (C—H = 0.95 Å) and were included in the refinement in the riding model approximation with U_{iso}(H) set to 1.2U_{eq}(C). The O- and N-bound H-atoms were located in a difference Fourier map and were refined with distance restraints of O—H = 0.84±0.01 Å and N—H = 0.88±0.01 Å, and with U_{iso}(H) = 1.2U_{eq}(N) and 1.5U_{eq}(O). Owing to being affected by the beam-stop, a reflection, *i.e.* (1 0 0), was omitted from the final cycles of refinement.

Computing details

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2005); cell refinement: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2005); data reduction: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

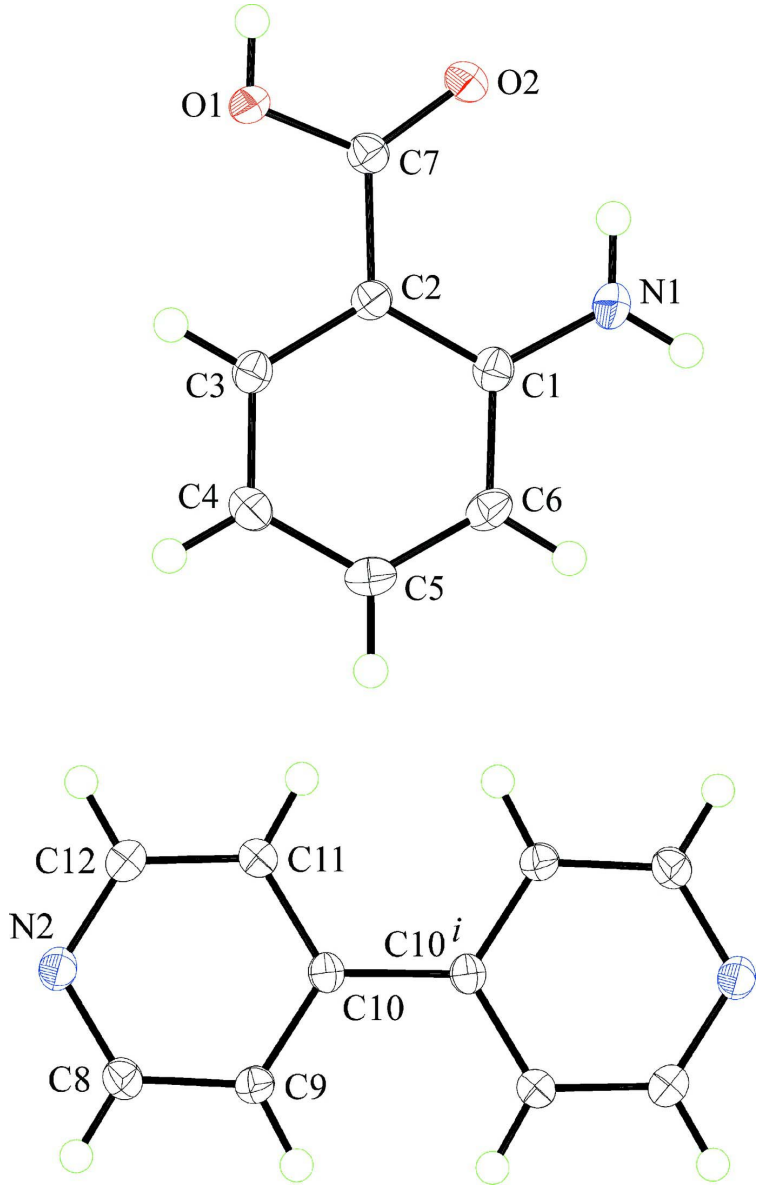

Figure 1

Molecular structures of the components of (I), showing atom-labelling scheme and displacement ellipsoids at the 50% probability level: (upper) 2-aminobenzoic acid and (lower) 4,4′-bipyridine. For symmetry code (i): -*x* + 1, -*y* + 1, -*z* + 1.

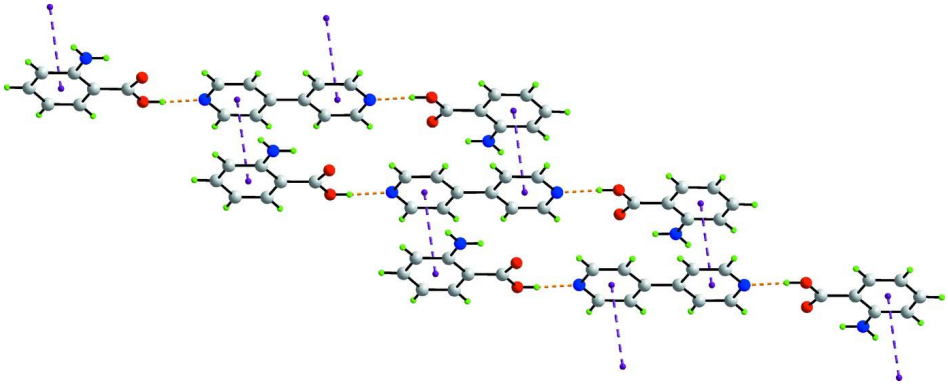

Figure 2

Detail of the π—π interactions between three-molecule aggregates in (I). The O—H···N and π—π interactions are shown as orange and purple dashed lines, respectively.

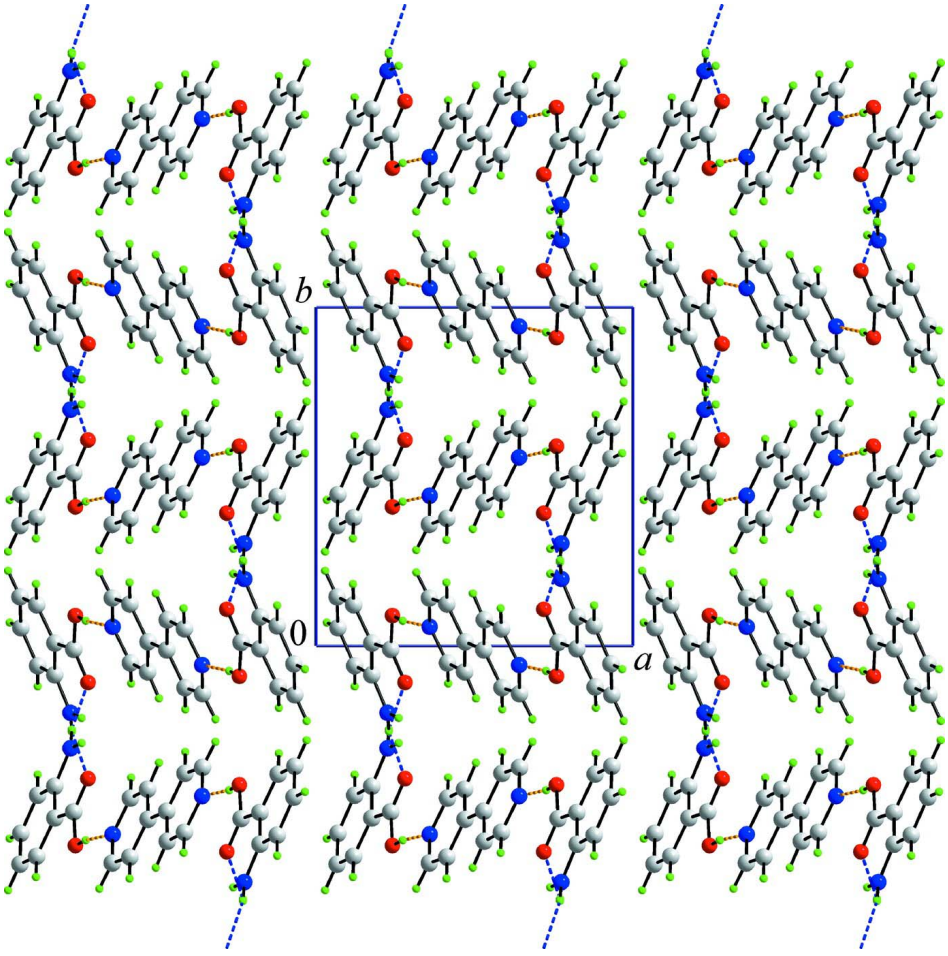

Figure 3

Unit-cell contents of (I) viewed in projection down the *c* axis. The N—H···O hydrogen bonds are shown blue dashed lines.

2-Aminobenzoic acid–4,4′-bipyridine (2/1)

Crystal data

$C_{10}H_8N_2·2C_7H_7NO_2$
M_r = 430.46
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 10.782 (5) Å
b = 10.998 (5) Å
c = 8.951 (4) Å
β = 107.215 (7)°
V = 1013.9 (8) Å^3
Z = 2
$F(000)$ = 452
D_x = 1.410 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71069 Å
Cell parameters from 3691 reflections
θ = 2.0–40.7°
μ = 0.10 mm^{-1}
T = 98 K
Prism, yellow
0.46 × 0.11 × 0.09 mm

Data collection

Rigaku AFC12K/SATURN724 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.723, T_{max} = 1.000
7849 measured reflections
2320 independent reflections
1932 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 27.5°, θ_{min} = 2.7°
h = −13→13
k = −14→14
l = −11→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.159
S = 1.11
2320 reflections
154 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0786P)^2 + 0.3371P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.24135 (13)	0.41046 (12)	0.79067 (14)	0.0227 (3)
H1O	0.277 (2)	0.426 (2)	0.8863 (13)	0.034*
O2	0.28109 (13)	0.60804 (12)	0.76583 (14)	0.0227 (3)
N1	0.22588 (18)	0.69761 (15)	0.47292 (19)	0.0275 (4)

H1N	0.264 (2)	0.711 (2)	0.5733 (11)	0.041*
H2N	0.233 (2)	0.7512 (18)	0.4034 (19)	0.041*
N2	0.35899 (15)	0.44351 (14)	0.09341 (17)	0.0204 (4)
C1	0.17630 (16)	0.58551 (17)	0.4277 (2)	0.0190 (4)
C2	0.17652 (16)	0.49167 (16)	0.53666 (19)	0.0174 (4)
C3	0.11939 (16)	0.37885 (17)	0.4823 (2)	0.0185 (4)
H3	0.1171	0.3173	0.5558	0.022*
C4	0.06660 (17)	0.35534 (18)	0.3247 (2)	0.0216 (4)
H4	0.0291	0.2784	0.2897	0.026*
C5	0.06951 (17)	0.44668 (19)	0.2180 (2)	0.0225 (4)
H5	0.0343	0.4312	0.1092	0.027*
C6	0.12234 (18)	0.55891 (17)	0.2671 (2)	0.0211 (4)
H6	0.1225	0.6196	0.1916	0.025*
C7	0.23616 (16)	0.51026 (16)	0.7065 (2)	0.0183 (4)
C8	0.35778 (17)	0.35879 (17)	0.2006 (2)	0.0209 (4)
H8	0.3171	0.2831	0.1659	0.025*
C9	0.41319 (17)	0.37652 (16)	0.3599 (2)	0.0190 (4)
H9	0.4122	0.3129	0.4313	0.023*
C10	0.47043 (16)	0.48801 (16)	0.41530 (18)	0.0163 (4)
C11	0.46902 (18)	0.57685 (17)	0.3028 (2)	0.0210 (4)
H11	0.5050	0.6549	0.3341	0.025*
C12	0.41485 (17)	0.55033 (18)	0.1457 (2)	0.0225 (4)
H12	0.4174	0.6110	0.0712	0.027*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0326 (7)	0.0183 (7)	0.0149 (6)	−0.0019 (6)	0.0036 (5)	0.0017 (5)
O2	0.0302 (7)	0.0181 (7)	0.0193 (6)	−0.0021 (6)	0.0065 (5)	−0.0038 (5)
N1	0.0423 (10)	0.0171 (8)	0.0225 (8)	−0.0046 (7)	0.0087 (7)	0.0027 (6)
N2	0.0229 (7)	0.0210 (8)	0.0167 (7)	0.0022 (6)	0.0048 (6)	0.0001 (6)
C1	0.0198 (8)	0.0165 (9)	0.0216 (9)	0.0025 (7)	0.0076 (7)	0.0007 (7)
C2	0.0198 (8)	0.0162 (9)	0.0167 (8)	0.0026 (7)	0.0064 (7)	0.0002 (6)
C3	0.0193 (8)	0.0168 (9)	0.0197 (8)	0.0015 (7)	0.0061 (7)	0.0015 (6)
C4	0.0211 (8)	0.0195 (9)	0.0227 (9)	−0.0018 (7)	0.0043 (7)	−0.0028 (7)
C5	0.0219 (9)	0.0276 (10)	0.0164 (8)	0.0031 (8)	0.0030 (7)	−0.0002 (7)
C6	0.0246 (9)	0.0213 (9)	0.0176 (8)	0.0056 (7)	0.0066 (7)	0.0037 (7)
C7	0.0198 (8)	0.0173 (9)	0.0185 (8)	0.0013 (7)	0.0065 (7)	−0.0016 (6)
C8	0.0239 (9)	0.0186 (9)	0.0197 (8)	0.0004 (7)	0.0059 (7)	−0.0024 (7)
C9	0.0227 (8)	0.0163 (9)	0.0179 (8)	0.0010 (7)	0.0056 (7)	0.0011 (6)
C10	0.0155 (8)	0.0182 (9)	0.0156 (8)	0.0009 (7)	0.0053 (6)	−0.0015 (6)
C11	0.0254 (9)	0.0186 (9)	0.0185 (8)	−0.0040 (7)	0.0054 (7)	−0.0012 (7)
C12	0.0259 (9)	0.0226 (9)	0.0184 (8)	−0.0008 (8)	0.0054 (7)	0.0026 (7)

Geometric parameters (Å, º)

O1—C7	1.323 (2)	C4—C5	1.393 (3)
O1—H1O	0.845 (10)	C4—H4	0.9500
O2—C7	1.233 (2)	C5—C6	1.376 (3)
N1—C1	1.357 (2)	C5—H5	0.9500

N1—H1N	0.882 (9)	C6—H6	0.9500
N1—H2N	0.876 (9)	C8—C9	1.387 (2)
N2—C12	1.340 (3)	C8—H8	0.9500
N2—C8	1.341 (2)	C9—C10	1.396 (3)
C1—C6	1.412 (2)	C9—H9	0.9500
C1—C2	1.420 (2)	C10—C11	1.400 (2)
C2—C3	1.407 (3)	C10—C10^{i}	1.484 (3)
C2—C7	1.479 (2)	C11—C12	1.385 (2)
C3—C4	1.380 (2)	C11—H11	0.9500
C3—H3	0.9500	C12—H12	0.9500

C7—O1—H1O	109.8 (17)	C5—C6—H6	119.4
C1—N1—H1N	118.5 (15)	C1—C6—H6	119.4
C1—N1—H2N	120.5 (15)	O2—C7—O1	122.21 (16)
H1N—N1—H2N	120.1 (16)	O2—C7—C2	123.99 (16)
C12—N2—C8	117.25 (15)	O1—C7—C2	113.76 (15)
N1—C1—C6	119.95 (16)	N2—C8—C9	123.08 (17)
N1—C1—C2	122.33 (16)	N2—C8—H8	118.5
C6—C1—C2	117.72 (17)	C9—C8—H8	118.5
C3—C2—C1	119.46 (15)	C8—C9—C10	119.95 (16)
C3—C2—C7	119.36 (15)	C8—C9—H9	120.0
C1—C2—C7	121.18 (16)	C10—C9—H9	120.0
C4—C3—C2	121.65 (16)	C9—C10—C11	116.62 (16)
C4—C3—H3	119.2	C9—C10—C10^{i}	122.0 (2)
C2—C3—H3	119.2	C11—C10—C10^{i}	121.4 (2)
C3—C4—C5	118.65 (18)	C12—C11—C10	119.66 (17)
C3—C4—H4	120.7	C12—C11—H11	120.2
C5—C4—H4	120.7	C10—C11—H11	120.2
C6—C5—C4	121.28 (17)	N2—C12—C11	123.39 (17)
C6—C5—H5	119.4	N2—C12—H12	118.3
C4—C5—H5	119.4	C11—C12—H12	118.3
C5—C6—C1	121.18 (16)		

N1—C1—C2—C3	177.74 (16)	C1—C2—C7—O2	5.0 (3)
C6—C1—C2—C3	−2.4 (2)	C3—C2—C7—O1	6.9 (2)
N1—C1—C2—C7	−2.5 (3)	C1—C2—C7—O1	−172.86 (16)
C6—C1—C2—C7	177.36 (15)	C12—N2—C8—C9	−1.2 (3)
C1—C2—C3—C4	2.2 (3)	N2—C8—C9—C10	1.9 (3)
C7—C2—C3—C4	−177.63 (16)	C8—C9—C10—C11	−0.5 (3)
C2—C3—C4—C5	−0.6 (3)	C8—C9—C10—C10^{i}	179.24 (19)
C3—C4—C5—C6	−0.7 (3)	C9—C10—C11—C12	−1.3 (3)
C4—C5—C6—C1	0.3 (3)	C10^{i}—C10—C11—C12	178.92 (19)
N1—C1—C6—C5	−178.94 (17)	C8—N2—C12—C11	−0.7 (3)
C2—C1—C6—C5	1.2 (3)	C10—C11—C12—N2	2.0 (3)
C3—C2—C7—O2	−175.22 (16)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1n···O2	0.88 (1)	2.02 (2)	2.697 (2)	132 (2)
O1—H1o···N2^{ii}	0.85 (1)	1.81 (1)	2.655 (2)	174 (2)
N1—H2n···O2^{iii}	0.88 (2)	2.14 (2)	3.002 (3)	170 (2)

Symmetry codes: (ii) *x*, *y*, *z*+1; (iii) *x*, −*y*+3/2, *z*−1/2.